Electronic levels of **free radicals.** B. N. Shvarts and M. B. Dyatkina (A. S. Pushkin State Pedagog. Inst., Bres?). Zhur. Fiz. Khim. 30, 432-5? (1956).—The electronic levels of phenylmethyl were calcd. by the valency bond and mol. orbital methods. The presence of an unpaired π-electron in the free radical conjugated bond system is responsible for the strong bathochromic effect, which offers an explanation for the appearance of color in the colorless aryl-substituted ethanes upon their dissocn. into free radicals. The electronic terms of vinylmethyl, divinylmethyl and trivinyl-methyl were calcd. by both quantum chem. methods. The calcns. have confirmed the experimentally observed rule of a shift in absorption toward the longer wave lengths on enlarging the conjugated bond system. The unpaired π-electrons in the conjugated bond system cause considerably greater bathochromic effect than an increase in the no. of conjugated bonds.

W. M. Sternberg

SHIRMAZAN, M.G.; DYATKINA, M.Ye.

New hybridization for the coordination number 9 and structure of
tricyclopentadienyluranium, Zhur. neorg. khim. 2 no.8:1761-1762
Ag '57.   (MIRA 11:3)
              (Stereochemistry)   (Uranium compounds)

ДУАТКINA, M. Ye.

AUTHOR: Dyatkina, M. Ye. (Moscow)

TITLE: Investigation of the Nature of Chemical Bonds and Atom Valences in
             Inorganic Compounds by the K-Absorption Edges in X-ray Spectra
             (Issledovaniya kharaktera khimicheskikh svyazey i valentnosti atomov
             v neorganicheskikh soyedineniyakh po K-krayam pogloshcheniya v
             rentgenovskikh spektrakh)

ABSTRACT: The problems most important in the theory of formation of inorganic
             compounds are discussed. The explanation of these problems is im-
             portant for the purpose of establishing the nature of the bonds be-
             tween the central atom and the addenda in complex compounds. A new
             method - study of the position and thin structure of the K-edge of
             x-ray absorption spectra of atoms in molecules - and its application
             are described. The K-edge of absorption corresponds to ionization
             as a result of electron separation from the atom. This method allows
             the orientation of levels to be investigated even in individual
             atoms. The thin structure at the K-edge of the absorption spectrum
             represents the essential characteristic of the atom or ion making

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Investigation of the Nature of Chemical Bonds and Atom Valences in
Inorganic Compounds by the K-Absorption Edges in X-ray Spectra

it possible to identify the atom or ion. The presence of absorption
in the field of low energies indicates that the substances investi-
gated possess approximately neutral atoms with blank orbits; because,
if these orbits would have been occupied by electrons there could
have been no absorption. The application of the x-ray spectra
method opens a way to the solution of problems regarding the nature
of bonds in amino complexes. Results obtained by this new method,
by foreign researchers, are listed.

There are 17 references, of which 4 are Slavic

ASSOCIATION:

PRESENTED BY:

SUBMITTED:

AVAILABLE:

Card 2/2

DYATKINA, M. YE.

AUTHORS: Dyatkina, M. Ye., Shustorovich, Ye. M.   20-6-28/47

TITLE: The Molecular Orbits of Systems Made up of Condensed Five-, Six- and Seven-Member Rings (Molekulyarnyye orbity sistem iz kondensirovannykh pyati-, shesti-i semichlennykh kolets)

PERIODICAL: Doklady AN SSSR, 1957, Vol. 117, Nr 6, pp. 1021-1022 (USSR)

ABSTRACT: The authors are interested in the molecular orbits of the systems of 3 condensed rings with five- and seven-member cycles and the calculated the energies of the molecular orbits of such systems by the usual method in the approximation ЛКАО. The results of calculation expressed by the Coulombian integrals C and by the resonance-integrals β are given in a table, where the energies of all suitable and also of the two lowest unsuitable molecular orbits are given. The authors' calculations confirm a conclusion of Dewar and Petitt (reference 3, 4). In different systems, according to these calculations, the number of suitable molecular orbits is equal to the number of the existing pairs of π-electrons, so that such systems must exist in the form of neutral molecules, Structural formulae with double bonds and with all tetravalent C-atoms may be ascribed to them. In a certain system

Card 1/2

The Molecular Orbits of Systems Made up of Condensed   20-6-28/47
Five-, Six- and Seven-Member Rings

with 11 π-electrons 6 suitable orbits exist, so that such a
condensed system must be inclined to the addition of an
excess electron under formation of $C_{11}H_{11}^{-}$. The pentanyl,
however, has no such inclination. But in another system only
7 suitable molecular orbits and 15 π-electrons exist, so
that the cycle $C_{16}H_{16}$ in the form of a single-charged cation
must be stable. The results for two of the systems investigated
here are called especially interesting. In the first one of
those the authors found 6 suitable molecular orbits so that
lo π-electrons exist. Therefore the cycle $C_{10}H_{10}$ is supposed
to be inclined to the addition of 2 excess electrons under
formation of a double-charged anion. In the second case of
special interest 16 π-electrons and only 7 suitable molecular
orbits exist, so that such a system must be inclined to
giving off 2 electrons with transition to a double-charged
cation. Therefore such a condensed system is supposed to con-
sist of three seven-member rings in the form of the salt
$(C_{16}H_{16})^{2+}x^{2-}$. There are 1 table, and 4 references, 0 of

Card 2/3   which are Slavic.

Inst. Gen. v Inorganic Chem im N. S. Kurnakov, AS USSR

ZEYEL', Frits [Seel, Fritz], prof., doktor; DYATKINA, M.Ye., doktor
    khim.nauk [translator]; ZAKHAR'YEVSKIY, V.A., red.; GRIBOVA,
    M.P., tekhn.red.

    [Atomic structure and chemical bonds; an introduction to
    the present-day theory of chemical bonds represented by
    visual aids] Stroenie atoma i khimicheskaia sviaz';
    vvedenie v sovremennuiu teoriiu khimicheskoi sviazi na
    osnove nagliadnykh predstavlenii. Moskva, Izd-vo inostr.
    lit-ry, 1958. 66 p. [Translated from the German]
                                            (MIRA 12:6)
                (Chemical bonds)

AUTHOR: Dyatkina, M. Ye.   SOV/78-3-9-7/38

TITLE: On the Electron Structure in the Compounds of Platinum With
Ethylene (Elektronnoye stroyeniye soyedineniy platiny s etilenom)

ABSTRACT: In the present paper the structure of the compound $(C_2H_4PtCl_4)^-$
was investigated with respect to its electron structure. In the
compound $(C_2H_4PtCl_3)^-$ the platinum state is d^9s_p. The three
bindings of platinum with chlorine atoms are formed at the ex-
pense of the atom orbits d_{z^2} and p_y. Apart from that, two donor-
acceptor bindings are formed. These donor-acceptor bindings can
be regarded as three centered orbits that are occupied by elec-
tron pairs. In the cis-compound $(C_2H_4)_2PtCl_2$ a double bond with
chlorine atoms is possible at the expense of an s- and a d-
orbit and 4 donor-acceptor bindings with 2 ethylene molecules.
In the trans-compound $(C_2H_4)_2PtCl_2$ the formation of a double
bond with two chlorine atoms and two donor-acceptor bindings

Card 1/2

On the Electron Structure in the Compounds of Platinum With Ethylene   SOV/78-3-9-7/38

at the expense of π-electrons with two ethylene molecules is only possible if the d-electron of platinum is excited to the p-orbits and a d-orbit is released. In the cis-compound $(C_2H_4)_2PtCl_2$, in contrast to the trans-compound, the formation of 4 donor-acceptor bindings between two ethylene molecules and one atom of platinum is possible, and it is stable. The results explain the lower stability of the trans-compounds as compared to the cis-isomers. There are 3 figures, 4 tables, and 3 references, 2 of which are Soviet.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii imeni N. S. Kurnakova, Akademii nauk SSSR (Institute of General and Inorganic Chemistry imeni N. S. Kurnakov, AS USSR)

SUBMITTED: July 11, 1957

Card 2/2

AUTHORS: Shustorovich, Ye. M., Dyatkina, M. Ye.   SOV/78-3-12-20/36

TITLE: I. The Valence State of the Elements of the First Transition
                Period in Bi-Cyclopentadienyl Compounds (I. Valentnyye
                sostoyaniya elementov pervogo perekhodnogo perioda v bis-
                tsiklopentadienil'nykh soyedineniyakh)

PERIODICAL: Zhurnal neorganicheskoy khimii, 1958, Vol 3, Nr 12,
                pp 2721-2735 (USSR)

ABSTRACT: In the present work a systematic calculation was made for the
                energies of the valence states of the first transition period
                elements (from Sc to Ni) in bis-cyclopentadienyl compounds
                (several valence states were calculated for each atom) using
                the method of (Slater) Sleyter-Kondor . In the molecules of
                these compounds exist the following bonds: unpaired electrons
                in the e_{1g} orbit and $d_{xz}d_{yz}$ orbits of the metals; electron
                pairs in the a_{1x}, a_{2u}, e_{1u} orbits and in the free orbits of the
                corresponding metals, s, p_z, p_x, p_y; electron pairs in the
                $d_{x^2-y^2}$, d_{xy} and free e_{2g} orbits. The relatively low energy of

Card 1/2   the valence state of the Ti^+ and V^{2+} permits the formation of

SOV/78-3-12-20/36

I. The Valence State of the Elements of the First Transition Period in Bi-
Cyclopentadienyl Compounds

the compounds $(C_5H_5)_2 Ti^+$ and $(C_5H_5)_2 V^{2+}$, but e_{2g} bonds are
lacking in these compounds. From the results obtained it is
possible to explain the difference in the properties of the
scandium compounds and those compounds of Ti^+ and V^{2+}, which
have a corresponding number of electrons. It is also possible
to explain the diamagnetic properties of $(C_5H_5)_2 Ti$, the

paramagnetism of $(C_5H_5)_2 V'$, the magnetic properties of $(C_5H_5)_2$
Mn and $(C_5H_5)_2 Fe^+$, the diamagnetism of ferrocene, the in-
stability of $(C_5H_5)_2 Ni$, and the formation of ring compounds
of Cu with cyclopentadienyl. There are 2 tables and 14 ref-
erences, 2 of which are Soviet.

SUBMITTED: October 10, 1957

Card 2/2

AUTHOR: Dyatkina, M. Ye.   SOV/78-3-12-36/36

TITLE: Concerning the Problem of the Structure of the Carbonyl Halides of Platinum (K voprosu o stroyenii karbonilgalogenidov platiny)

ABSTRACT: The work of Irving and Magnusson showing the peculiarity of the compound $Pt.CO.Hal_2$ was discussed. The platinum atom is bonded with the CO addenda through π-bonds and is not directly bound through the carbon atoms. The halogens are bonded by two normal covalent bonds and a donor-acceptor bond. The CO group is perpendicular to the plane in which the Pt and halogen atoms are found. Similar structural representations were made for other carbonyl compounds and for compounds with other groups which contain π-bonds, as, for example, nitrosyl compounds. In $Pt(NH_3)_4(CN_3CN_2)$ the molecular group CN_3CN is bonded to the platinum atom by the $C \equiv N$ bond and not through the nitrogen atoms. There are 5 references, 2 of which are Soviet.

Card 1/2

AUTHORS: Shirmazan, M. G. , Dyatkina, M. Ye.   SOV/62-58-7-19/26

TITLE: On the Problem Concerning the Structure of the $Mo(CN)_8^{4-}$ Ion
                (K voprosu o stroyenii iona $Mo(CN)_8^{4-}$)

PERIODICAL: Izvestiya Akademii nauk SSSR, Otdeleniye khimicheskikh nauk,
                1958, Nr 7, pp. 898-899 (USSR)

ABSTRACT: In one of the previous papers (Ref 1) the authors discussed
                already the maximum values (znacheniya) of the functions
                (as well as the angles between the directions of the maximum
                values) calculated for hybrid atomic orbits in the case of
                coordination numbers of 2 - 9, among them also for the co-
                ordination number 8. It was shown that in the hybridization
                of d^4sp^3 electrons 8 hybrid orbits of great maximum values
                (symmetry D_{2d}) can develop, which would correspond to a
                configuration exhibited by the $Mo(CN)_8^{4-}$ ion. Dyukyulo (Ref 2)
                deals with the same problem, however, he concludes that in
                the hybridization of the d^4sp^3 electrons only relatively
                weak bonds can be formed. According to the opinion of the
                authors Dyukyulo arrived at that conclusion because of the
Card 1/2   method employed by him (composition of hybrid orbits). In

On the Problem Concerning the Structure of the $Mo(CN)_8^{4-}$ Ion   SOV/62-58-7-19/26

the present paper the authors prove that a dodecahedral structure is also possible without a removal of f-electrons. There are 2 references, 1 of which is Soviet.

ASSOCIATION: Institut tonkoy khimicheskoy tekhnologii im. M. V. Lomonosova (Institute of Fine Chemical Technology imeni M. V. Lomonosov)

SUBMITTED: February 24, 1958

Card 2/2

AUTHOR: Dyatkina, M. Ye. (Moscow)   74-27-1-2/4

TITLE: Structure and Nature of the Compounds in Aromatic Complexes
               of Metals (Stroyeniye i priroda svyazey v aromaticheskikh
               kompleksakh metallov)

PERIODICAL: Uspekhi Khimii, 1958, Vol. 27, Nr 1, pp. 57-93 (USSR)

ABSTRACT: The problem of the nature of the chemical compounds in
               metal compounds with aromatic hydrocarbons is one of the
               most topical problems of the structure of molecules. The
               capability of the cyclopentadienyl group to produce compounds
               with other elements alone is not surprising. But on the other
               hand the C_5H_5-group can appear as an anion of $C_5H_5^-$ in
               chemical compounds, in which case ion bonds to cations of
               electropositive metals are developing. After introductory
               descriptions of the structure of the molecules referring to
               a few papers published in foreign countries the author deals
               with the geometry of the molecules. Table 1 gives radiographic
               data on the structure of several crystals of different in-
Card 1/3   vestigated compounds. Then the author occupies himself with

the molecules of ferrocene structure and with the problem
of the cyclopentadienyl rings: The possibility of the con-
figuration as a pentagonal prism, or as antiprism, or as a
configuration with free rotation of the rings round the
general axis. In detail the author deals with the electrono-
graphic investigations in this field. Moreover the author
deals with the energies of the bis-cyclopentadienyl compounds
of the metals. They are especially stable, which was con-
firmed by thermochemical investigations. It was referred to
the investigations by Lippencott and Nelson, their computations
of the thermodynamic functions which make it evident that
$(C_5H_5)_2$ belongs to the most stable ones, whereas $(C_5H_5)_2Ni$
is of the lowest stability. The mass spectra as additional
sources for finding out the energies of the substances under
question, especially of the bis-cyclopentadienyl compounds,
are mentioned, investigations of Friedman, Irsa and Wilkinson
are referred to (see table 2). The magnetic properties of
transition elements (perekhodnye) are especially considered.
Among other things the particular magnetic properties of

Card 2/3 $(C_5H_5)_2MN$ are discussed, as well as those of the tricyclo-

Structure and Nature of the Compounds in Aromatic Complexes   74-27-1-2/4
of Metals

pentadienyls of the rare earth elements. In special para-
graphs the author deals with the oscillation- and electronic
absorption spectra and with the results of the investigation
of $(C_5H_5)_2Fe$, $(C_5H_5)_2Ru$, $(C_5H_5)_2Ti(CH_3)_2$, of which infrared
spectra as well as spectra of the combination scattering were
obtained. Moreover the author discusses the investigations
carried out by Kauer (absorption spectra of the x-rays),
furthermore the chemical properties of the bi-cyclopenta-
dienyl compounds and the characteristics of the bonds. On
account of the facts discussed the author comes to the
conclusion that there are different types of cyclopentadienyl
compounds of the metals which differ from each other by their
type of compound. Furthermore the author deals with the
aromatic character of the bi-cyclopentadienyl compounds and
the nature of the compounds in aromatic complexes of the
metals. There are 8 figures, 6 tables, and 83 references,
6 of which are Soviet.

Card 3/3   1. Cyclic compounds--Structural analysis

5(4)

AUTHORS: Dyatkina, M. Ye., Syrkin, Ya. K.,   SOV/20-122-5-25/56
              Corresponding Member, Academy of Sciences, USSR

TITLE: The Three-Center Orbits and the Structure of Cyclo-
              propane and Other Compounds With Three-Member Rings
              (Trekhtsentrovyye orbity i stroyeniye tsiklopropana i
              drugikh soyedineniy s trekhchlennymi kol'tsami)

ABSTRACT: According to the results obtained by various previous
              papers (Refs 1,2,3) the formation of three-center
              orbits is not a special case and occurs rather frequently
              in the case of various molecules. Such orbits may,
              according to the authors' opinion, exist in a far
              greater number of cases that hitherto assumed. By
              utilizing the ideas concerning three-center orbits
              it is possible to explain the structure of various
              molecules. This is the case especially with a number
Card 1/2   of compounds with an insufficient number of electrons,

The Three-Center Orbits and the Structure of Cyclo-
propane and Other Compounds With Three-Member Rings

SOV/20-122-5-25/56

which are formed by the attachment of a proton
to the valence-saturated molecules. For H_3^+ only the
hypothesis of the existence of three-center orbits
is of use. The author believes that something similar
applies also to CH_5^+. Three-center orbits are probably
possible also in molecules with three-member
cycles. It is just this special configuration of a three-
member ring with angles of $60°$ that is indicative of a
possible realization of three-center orbits also
in this case. The authors then dwell somewhat more
in detail upon this hypothesis, which is suited
not only for cyclopropane but also for various of its
analogues.(e.g.ethylene oxide and ethylenimide). Its
may also be possible that three-center orbits form
the basis of $Fe_3(CO_3)_{12}$. There are 5 figures and 8
references, 3 of which are Soviet.

SUBMITTED: July 7, 1958

Card 2/2

5(4)

AUTHORS: Dyatkina, M. Ye., Dobryakov, S. N.,   SOV/20-123-2-28/50
                Shustorovich, Ye. M.

TITLE: The Molecular Orbits of Radicals With Non-Alternant Cycles
                (Molekulyarnyye orbity radikalov s neal'ternantnymi tsiklami)

PERIODICAL: Doklady Akademii nauk SSSR, 1958, Vol 123, Nr 2, pp 308-311
                (USSR)

ABSTRACT: The authors first discuss the characteristic features of
                systems with non-alternant cycles which were determined by an
                earlier paper (Ref 1). These results induced the authors to in-
                vestigate also other compounds with five- and seven- membered
                cycles, namely radicals which are analogous to diphenyl methyl
                and dinaphtyl methyl with cyclopentadienyl-, cycloheptatrienyl-,
                and azulenyl residues. Calculations were carried out by the
                simplified method of molecular orbits under usual conditions.
                The systems investigated are given in a table, where also
                the number of connecting (svyazyvayushchiy), non-connecting
                (nesvyazyvayushchiy), and separating (razrykhlyayushchikh)
                levels of these molecules are mentioned. Various details con-
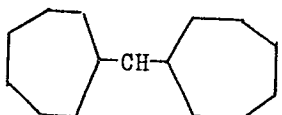   cerning these systems are given; the following conclusions may
Card 1/3   be drawn:

The Molecular Orbits of Radicals With Non-Alternant   SOV/20-123-2-28/50
Cycles
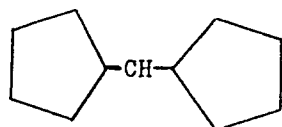
must, like the radical cyclopentadienyl,

be stable in form of a singly charged anion, and

in form of a singly charged cation, as

e.f. tropyl. In the same way also such systems must behave in
which, apart from the non-alternant ring, also a condensed
6-membered ring exists. The radicals with heptalinyl rests have
a non-connecting level. Finally, some structural common
features and differences between the structure of the systems
listed in the table are pointed out. There are 1 table and 3
references, 2 of which are Soviet.

Card 2/3

5(4)

AUTHORS: Dyatkina, M. Ye., Shustorovich, Ye, M.   SOV/78-4-2-25/40

TITLE: The Valence States of the Central Atoms in Aromatic Complexes
               of Metals (Valentnyye sostoyaniya tsentral'nykh atomov v
               aromaticheskikh kompleksakh metallov)

ABSTRACT: The valence state of the central atoms in aromatic complex
               compounds of the type $(C_6H_6)_2Me$ (Me = V^+, V, Cr^+, Cr, Mo,
               and Fe^{++}) is discussed. The excitation energies of the basic
               state and of the various valence states of the configurations
               d^4, s^2d^3, d^5 and d^6 are shown in detail in table 1. Considering
               the excitation energies in the various valence states, the
               diamagnetic properties of dibenzene chromium, dibenzene
               molybdenum, and of divalent dibenzene iron can be explained.
               The excitation energies were calculated on account of the
               valence state of the individual atoms and are shown in table 2.
               The energy of the individual combinations in the compounds of
               the type dibenzene-chromium can be calculated from the

Card 1/2

The Valence States of the Central Atoms in Aromatic Complexes of Metals   SOV/78-4-2-25/40

energies of the various valence states. The donor-acceptor functions between the electronic couples of the benzene cycle and the free orbitals of the central atom, sa_{1g} and $de\pm_{1g}$ are decisive in the case of these compounds. There are 2 tables and 6 references, 2 of which are Soviet.

SUBMITTED: November 1, 1957

Card 2/2

5(4)

AUTHORS: Shustorovich, Ye. M., Dyatkina, M. Ye,   SOV/78-4-3-11/34

TITLE: The Valence States of the Central Atoms in the Aromatic
                Complexes of Metals (Valentnyye sostoyaniya tsentral'nykh
                atomov v aromaticheskikh kompleksakh metallov)

ABSTRACT: In the formation of bis-cyclopentadienyl compounds of the
                elements of the second and third transition periods the
                valence state is similar to that of the elements of the first
                transition period and is characterized by odd electrons in

                shells d_{xz}, d_{yz} $(e_{1g}^{\pm})$. The difference between the excitation
                energies of Fe (110 kcal) and Ru (35-37 kcal) in a corresponding
                valence state is responsible for the higher stability of
                ruthenocene compared to ferrocene. In view of the magnitude
                of the energy of $(C_5H_5)_2Zr$ this compound is believed to be
                diamagnetic. 61 kcal (instead of 82 kcal with titanium) are

Card 1/3   required to excite the d^4 configuration in zirconium. For

The Valence States of the Central Atoms in the Aromatic   SOV/78-4-3-11/34
Complexes of Metals

this reason the bonds for forming bis-cyclopentadienyl
compounds are more favorable in zirconium than in titanium.
The difference between the energy of the valence states

$d_{xz}d_{yz}d^+_{x^2-y}2d^+_{z^2}$ and $d_{xz}d_{yz}d^2_{x^2-y}2$ is 12 kcal. A comparison has
shown that the energy of the valence state of rhenium is lower
than that of manganese. The energy required for exciting

rhenium d^7 is 72 kcal, for manganese d^7 it is 132 kcal. The
energy difference is one of the main causes for the difference
in properties between manganese and rhenium. Manganese does
not form compounds, rhenium forms the compound $(C_6H_6)_2Re^+$.

The excitation energies of Mn and Re in a corresponding
valence state have not been compared because there are no data
on the rhenium spectra. The excitation energy in the

d^3 configuration of yttrium is near that of scandium (97 kcal)
and amounts to 84 kcal. In the case of yttrium and scandium,
ionogenic tricyclopentadienide is formed. The valence states
Card 2/3   in the cyclopentadienyl compounds of nickel, palladium,and

The Valence States of the Central Atoms in the Aromatic SOV/78-4-3-11/34
Complexes of Metals

platinum have been discussed. Palladium shows the initial
state d^9p with an excitation energy of 110 kcal. Platinum has
the valence state d^9s and differs from the initial states of
nickel and palladium. This state is favorable for combining
the platinum atom with 2 chlorine atoms and 2 ethylene
molecules in cis-configuration. The structure of platinum
cyclopentadienyl in the initial state has electron
configurations which favor the formation of donor-acceptor
bonds and dative bonds with two double bonds. There are
9 references, 3 of which are Soviet.

SUBMITTED: December 23, 1957

Card 3/3

5(4)

AUTHORS: Dyatkina, M. Ye., Syrkin, Ya. K.

SOV/78-4-6-12/44

TITLE: On the Problem of the Stereochemistry of the Bimolecular
Substitution in Complex Compounds (K voprosu o stereokhimii
bimolekulyarnogo zameshcheniya v kompleksnykh soyedineniyakh)

PERIODICAL: Zhurnal neorganicheskoy khimii, 1959, Vol 4, Nr 6, pp 1285-1290
(USSR)

ABSTRACT: The stereochemistry of the bimolecular substitutions in octa-
hedral and quadratic complexes was investigated. It was found
that in the case of the transition of the configuration of
the complex from the quadratic to the bipyramidal one a
substitution of the addends occurs as well as a change of
the valence state of the central atom. In the case of the
bimolecular substitution in octahedral complexes it is possible
that the free orbits with greater principal quantum number
take part in the development for the production of complex
compounds with additional substitution groups. The intermediate
complexes with tetragonal pyramidal structure are important
in the kinetics of the reaction of the bi- and tetravalent
platinum. In the case of the substitution in complexes with
Card 1/2   quadratic configuration the formation reaction proceeds under

SOV/78-4-6-12/44

On the Problem of the Stereochemistry of the Bimolecular Substitution in Complex Compounds

formation of intermediate complex compounds with tetragonal and pyramidal configuration. There are 7 figures and 6 references, 3 of which are Soviet.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii im. N. S. Kurnakova Akademii nauk SSSR
(Institute of General and Inorganic Chemistry imeni N. S. Kurnakov of the Academy of Sciences, USSR)

SUBMITTED: March 25, 1958

Card 2/2

5(0)   SOV/30-59-6-2/40

AUTHORS: Syrkin, Ya. K., Corresponding Member, Academy of Sciences, USSR,
                Dyatkina, M. Ye., Doctor of Chemical Sciences

TITLE: The Present State of Quantum Chemistry (Sovremennoye
                sostoyaniye kvantovoy khimii)

ABSTRACT: The beginnings of quantum chemistry are to be found in the work
                by W. Heisenberg (1926) who investigated the first multi-elec-
                tron system - the helium atom - as well as in the work by
                Heitler and London who used the same method for investigating
                the hydrogen molecule H_2 (1927). In these investigations the

                physical reasons for the formation of a covalent bond were dis-
                covered for the first time, however, no accurate solution of
                the Schrödinger equation for these problems could be obtained.
                For this reason an approximation method had to be applied. It
                may be seen from it that in the near future it will hardly be
                possible to obtain reliable values in quantum chemistry of the
                dissociation energy by theoretical computations. Concerning
                the problems of a survey of the existing approximated and exact

Card 1/2

The Present State of Quantum Chemistry   SOV/30-59-6-2/40

methods of computation the authors of this article refer to the paper by P. Levdin (footnote 1). Furthermore, a number of interesting results obtained in the field of qualitative conclusions from chemical quantum computations are demonstrated, the values of which are acknowledged by the authors. The concepts concerning the directivity of valencies is regarded as a success of qualitative quantum chemistry. Chemical quantum computations of covalent atomic radii in condensated aromatic hydrocarbons also proved to be successful. The problem of the application of quantum-chemical methods for determining spectral properties of chemical compounds is also of interest. There are 1 figure and 1 reference.

Card 2/2

5 (4)

AUTHOR: Dyatkina, M. Ye.   SOV/62-59-6-11/36

TITLE: Molecular Orbits of Chromium-dibenzene (Molekulyarnyye orbity
             dibenzolkhroma)

PERIODICAL: Izvestiya Akademii nauk SSSR. Otdeleniye khimicheskikh nauk,
             1959, Nr 6, pp 1025 - 1027 (USSR)

ABSTRACT: The formation of the molecular orbits of chromium-dibenzene
             from the atomic orbits of Cr and that of the orbits of the
             two benzene molecules is regarded from the point of view of
             the group displacement law. Chromium-dibenzene was therefore
             taken for the investigation as with it, that is in benzene,
             there occur only orbits of paired electrons and no molecular
             orbits of unpaired electrons with electrons of the central
             atom. The problem is only qualitatively dealt with. With the
             following orbits a possible interaction was determined: the
             occupied orbit of the benzene molecule (B) of the symmetry
             a_{1g} with the 4s orbit of Cr (hydride orbit from 4s and $3dz^2$),
             the occupied orbit of B a_{2n} with $4p_z$, the occupied orbit of
             B e_{1g} with $3d_{xz}$, $3d_{yz}$ the occupied orbit of B e_{1n} with $4p_x$,

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Molecular Orbits of Chromium-dibenzene   SOV/62-59-6-11/36

$4p_y$ and the free orbit of B e_{2g} with $3d_{xy}$, $3d_{x^2-y^2}$. This corresponds to the formation of three donor-acceptor bonds at the expense of the occupation of the C H-orbit and the free d^2sp^3-orbits of Cr, and of one donor-acceptor bond at the expense of the occupied d_{xy}, $d_{x^2-y^2}$-orbits of Cr and the free orbit of C_6H_6. There are 9 references, 1 of which is Soviet.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii im. N. S. Kurnakova
(Institute of General and Inorganic Chemistry imeni N. S. Kurnakov)

SUBMITTED: September 11, 1957

Card 2/2

Shirmazan, M. G., Dyatkina, M. Ye.

TITLE: Studies of Directed Valences. Report 1. Direction and Maximum
           Value of Hybrid Orbitals for the Coordination Numbers 2, 3, 4

ABSTRACT: In the present paper an expression is found for the analytical
           calculation of the hybrid orbitals with the coordination num-
           bers 2, 3 and 4 and for the symmetries C_{2v}, $D_{\infty h}$, C_{3v}, T_d, C_{4v},
           and D_{4h}. On the basis of these analytical expressions it is
           possible to determine the direction of the maximum concentration
           and the maximum value of the hybrid orbitals. From the sum of
           the maximum values of these functions the question of the pos-
           sible existence of this or another symmetry can be solved. The
           angle between the directions of maximum concentration was de-
           termined for the symmetries from the various possible values of
           the valency angle. The symmetries are represented on the figures
           and the tables list the values of the angles. There are
Card 1/2   10 figures, 10 tables, and 5 references, 4 of which are Soviet.

SOV/62-59-9-7/40

Studies of Directed Valences. Report 1. Direction and Maximum Value of Hybrid Orbitals for the Coordination Numbers 2, 3, 4

ASSOCIATION: Institut obshchey i neorganicheskoy khimii im. N. S. Kurnakova Akademii nauk SSSR (Institute of General and Inorganic Chemistry imeni N. S. Kurnakov of the Academy of Sciences, USSR)

SUBMITTED: December 30, 1957

Card 2/2

SYRKIN, Ya.K.; DYATKINA, M.Ya., doktor khim. nauk

Current status of quantum chemistry. Vest. AN SSSR 29 no.6:13-25
Je '59.   (MIRA 12:5)

1.Chlen-korrespondent AN SSSR (for Syrkin).
    (Chemistry, Physical and theoretical) (Quantum theory)

5(3)

AUTHORS: Dyatkina, M. Ye., Poray-Koshits, M. A.   SOV/20-125-5-21/61

TITLE: A New Possible Type of Isomerism in the Octahedral
             Complexes of Some Transition Elements, Especially Cu
             (O novom vozmozhnom tipe izomerii v oktaedricheskikh
             kompleksakh nekotorykh perekhodnykh elementov, v
             chastnosti Cu)

PERIODICAL: Doklady Akademii nauk SSSR, 1959, Vol 125, Nr 5,
             pp 1030-1032 (USSR)

ABSTRACT: A cis-trans-isomerism is known to be possible in the
             complexes mentioned in the title, which contain at least
             two kinds of ligands. In the case of a "regular" octahedral
             structure only the aforementioned type of isomerism is to
             be expected except optical isomerism. However, the authors
             try to prove that in several cases additional types of
             isomerism of the aforesaid complexes may occur. According
             to modern conceptions concerning the field theory of
             ligands, distortions are bound to occur under certain
             circumstances in consequence of the Yan-Teller effect. This
             is really the case. This distortion is bound to occur along
             one of the oscillation coordinates. Recently several

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A New Possible Type of Isomerism in the Octahedral   SOV/20-125-5-21/61
Complexes of Some Transition Elements, Especially Cu

research workers used these assumptions for the explanation
of the distortion of the regular octahedral arrangement
of ligands around the central atom in the case of the
compounds of Cu (II), Cr (II), and Mn (III) (Refs 1, 2).
It has, however, hitherto been neglected that in the
presence of two types of ligands such distortions may
cause further types of spatial isomerism. In the case of a
tertragonal distortion the existence of two types is in
principle possible: a) one corresponds to an extended
octahedron, b) the other one to a compressed octahedron.
In principle such an isomerism may occur as well in the case
of six equal ligands. However, only distortions of the
type a) have hitherto been found to occur in the case of
equal ligands. An attempt was made (Ref 3) to explain this
fact theoretically. The number of possible isomers in the
case of the composition $AX_2Y_2Z_2$ (see Scheme) is assumed to
be the greatest. In the case of the type of distortion a)
and b) three isomers are possible for each. This depends

Card 2/4   on the fact which of the three couples of ligands lies on

A New Possible Type of Isomerism in the Octahedral   SOV/20-125-5-21/61
Complexes of Some Transition Elements, Especially Cu

the axis which differs from the other ones. The authors
assume that this very type of isomerism holds for the cases
(Ref 4) of $Cu(NH_3)_2Br_2$ and $Cu(NH_3)_2Cl_2$ with a coordination
polyhedron $Cu(NH_3)_2X_4$. It was assumed (Ref 1) that those
ligands that create a less intense field are bound to lie
on the long axes. According to the increasing field strength,
the ligands form a series $Br < Cl < H_2O < C_6H_5N < NH_3 < CH_2NH_2CH_2NH_2$
(Ref 6) so that water and especially ammonia have to tend
towards a position on a short axis, compared with bromine.
This agrees with the structure of the a-isomer and explains
why no b-isomer is produced. In the latter the ammonia
molecules would lie on the longer axis, contrary to the
greater strength of the field produced by them. The
probability of the formation of a compressed isomer b
increases with increasing difference of the field strength
which is produced by various ligands. The above-mentioned
data indicate that the isomerism of Cu (II) compounds
detected by Hanic (Ref 4) is not only based upon the

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A New Possible Type of Isomerism in the Octahedral   SOV/20-125-5-21/61
Complexes of Some Transition Elements, Especially Cu

difference between the quadratic dsp^2-(or sp^2d)-hybridization
and the linear sp-hybridization. The authors assume that all
six ligands lie in all cases in the "internal sphere"
around the copper atom. The existence of isomerism is due
to the distortion of the coordination octahedron in consequence
of the Yan-Teller effect. There are 1 figure and 6 references,
1 of which is Soviet.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii im. Kurnakova
Akademii nauk SSSR (Institute of General and Inorganic
Chemistry imeni Kurnakov of the Academy of Sciences,USSR)

PRESENTED: December 27, 1958, by I. I. Chernyayev, Academician

SUBMITTED: December 27, 1958

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5. 3100, 5. 3700 (B)   66434

-5 (4)

AUTHORS: Shustorovich, Ye. M., Dyatkina, M. Ye.   SOV/20-128-6-39/63

TITLE: The Molecular Orbits of Dibenzene Chromium, Ferrocene, and the
                Cobalticinium Cation $Co(C_5H_5)_2^+$

PERIODICAL: Doklady Akademii nauk SSSR, 1959, Vol 128, Nr 6, pp 1234 - 1237
                (USSR)

ABSTRACT: The authors start from the point of view that the electronic
                structure of aromatic metal complexes can be determined by the
                methods of molecular orbits (mo) only. Since M. Yamazaki (Ref 2)
                published the method for the quantitative calculation of the mo
                of ferrocene $Fe(C_5H_5)_2$ in 1956, the authors have been engaged
                in the calculation of the mo of dibenzene chromium $Cr(C_6H_6)_2$
                and the cobalticinium cation $Co(C_5H_5)_2^+$ as well as the checking
                of the data concerning ferrocene given by Yamazaki. The calcula-
                tions were made according to the method developed by C. C. J.
                Roothaan (Ref 3). It was assumed that the mo of these compounds
                are formed of the mo of the rings C_5H_5 and C_6H_6, respectively,
                (consisting of the 2pπ atomic orbits of the C-atoms) and the

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The Molecular Orbits of Dibenzene Chromium, Ferrocene,   SOV/20-128-6-39/63
and the Cobalticinium Cation $Co(C_5H_5)_2^+$

nine $3d^5 4s\ 4p^3$ atomic orbits of the central atom. Further, the
following simplifying conditions were assumed to hold for the
purpose of the calculation: 1) the 18 valency electrons of the
complex are found in the positive field of the central atomic
residue (Cr^{6+}, Fe^{8+}, Co^{9+}) and the residue of the C-rings in
which each of the C-atoms has a positive charge; 2) all 18 elec-
trons are represented by Slater wave functions (Table 1); 3) in
the matrix of non-orthogonality the non-diagonal terms $S_{i,j}$
($i \neq j$) equal zero; 4) in the calculation of the H_{ij} elements
of the matrix all resonance integrals between not neighboring
C-atoms were considered to equal zero, while for neighboring
C-atoms β_{CC} was assumed to equal 2.39 ev; 5) in the calculation
of the diagonal elements H_{ii} of the matrix corresponding to the
$2p\pi$ atomic orbits of the C-atoms the energy of the valency state
of the (W_{2p} = -11.28 ev) was considered as it is usually done
in the calculation of the π-electron system; 6) in the matrix

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The Molecular Orbits of Dibenzene Chromium, Ferrocene,   SOV/20-128-6-39/63
and the Cobalticinium Cation $Co(C_5H_5)_2^+$

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of the interaction of the electrons the integrals of the form

$$\int \frac{\varphi_i^2(1)\varphi_j^2(2)}{r_{12}} d\tau_1 d\tau_2$$ only were considered; 7) the interaction

of the $3d_{z^2}$ atomic orbits with the mo of the C-rings could be
neglected, as can be seen from the integrals of non-orthogonali-
ty given in table 2. The calculated energies of the mo are con-
tained in table 3. The distribution of the electron density and
the calculated effective charges of the individual atoms of the
molecules are given in table 4. In dibenzene chromium the
Cr-atom has a positive charge of 1.147, in ferrocene Fe a charge
of +.0.68, while in $Co(C_5H_5)_2^+$ the Co-atom is negatively charged
(-0.118). Thus, in $Cr(C_6H_6)_2$ there occurs a shift of the elec-
trons from the metal to the rings, while a dipole moment forms.
The same effect occurs to a less degree in the case of ferro-
cene. In the case of cobalticinium, however, the electrons are
Card 3/4   shifted from the rings to the central atom and compensate the

The Molecular Orbits of Dibenzene Chromium, Ferrocene, and the Cobalticinium Cation $Co(C_5H_5)_2^+$

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SOV/20-128-6-39/63

original positive charge of Co to such an extent that the positive charge of the cation complex seems to be distributed to the 10 C-atoms of the rings. There are 4 tables and 7 references, 2 of which are Soviet.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii Akademii nauk SSSR (Institute of General and Inorganic Chemistry of the Academy of Sciences, USSR)

PRESENTED: June 5, 1959, by I. I. Chernyayev, Academician

SUBMITTED: May 22, 1959

Card 4/4

SHUSTOROVICH, Ye.M.; DYATKINA, M.Ye.

Calculation of the ground state of the ferrocene molecule with
the aid of the molecular orbital method with self-consistency.
Zhur strukt. khim. 1 no.1:109-121 My-Je '60.   (MIRA 13:8)

1. Moskovskiy institut tonkoy khimicheskoy tekhnologii imeni
M.V. Lomonosova i Institut obshchey i neorganicheskoy khimii imeni
N.S. Kurnakova.
                    (Ferrocene)

AUTHORS: Dyatkina, M. Ye., Syrkin, Ya. K.

TITLE: Participation of d-Orbits in the Bonding of Atoms With s-
               and p-Electrons

PERIODICAL: Zhurnal neorganicheskoy khimii, 1960, Vol. 5, No. 8,
               pp. 1663-1668

TEXT: The authors studied the increased stability of single bonds between
equal atoms. These bonds constitute the simpler type of covalent bonds if
they are not complicated by a partially ionic character. But even these
bonds may have anomalities. Even in cases where atoms forming diatomic
molecules have only one unpaired electron, there is a number of deviations
from the simple distribution of energy in single bonds. All data confirm
the low stability of single bonds in alkali metals, oxygen, nitrogen,
and fluorine, and also increased stability of such bonds in elements of the
copper sub-group, in phosphorus, sulfur, chlorine, and their analogs. The
increased stability of single bonds between equal atoms of sulfur, phosphor,
chlorine, and their analogs, as well as of elements of the copper sub-group

Card 1/2

Participation of d-Orbits in the Bonding   S/078/60/005/008/019/031/XX
of Atoms With a- and p-Electrons   B023/B066

as compared with oxygen, nitrogen, fluorine, and alkali metals may be
explained by the participation of electron pairs and free d-orbits in
bonding. Electron pairs and free d-orbits may also take part in the inter-
molecular interaction in crystals and metallic compounds. Investigations
of the authors are not mentioned. There are 6 references: 2 Soviet, 1
Belgian, 1 German, and 2 US.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii im. N. S.
               Kurnakova Akademii nauk SSSR (Institute of General and
               Inorganic Chemistry imeni N. S. Kurnakov of the Academy of
               Sciences USSR)

SUBMITTED: April 24, 1959

Card 2/2

SHUSTOROVICH, Ye.M.; DYATKINA , M.Ye.(Moscow)

Computation of two-center molecular integrals including   orbitals.
Zhur. fiz. khim. 34 no.3:644-650 Mr '60.   (MIRA 13:11)

1. Institut tonkoy khimicheskoy tekhnologii imeni M.V.Lomonosova
Adademiya nauk SSSR i Institut obshchey i neorganicheskoy khimii
imeni N.S.Kurnakova.
                    (Molecular theory)

S/076/60/034/008/030/039/XX
B015/B063

AUTHORS: Shustorovich, Ye. M. and Dyatkina, M. Ye.

TITLE: Some Molecular Integrals With the Participation of 3d, 4s,
             and 4p Orbits

PERIODICAL: Zhurnal fizicheskoy khimii, 1960, Vol. 34, No. 8,
             pp. 1843-1846

TEXT: In Ref. 1, the authors had obtained general formulas for the calcula-
tion of the Coulomb integrals and of the integrals of electron attraction
by nuclei for any combination of Slater's atomic orbits. The representation
applied was similar to that of Roothaan (Ref. 2). In the present work, the
authors have derived equations for calculating integrals with the parti-
cipation of 3d, 4s, and 4p Slater atomic orbits. These equations were ob-
tained from calculations of the molecular orbits of aromatic metal com-
plexes of the metals of the first transition period of the periodic system.
The integrals of nuclear attraction and one-center Coulomb integrals are
exactly calculated, whereas simpler approximate equations are proposed
for the two-center Coulomb integrals. Some two-center Coulomb integrals

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Some Molecular Integrals With the Participation S/076/60/034/008/030/039/XX
of 3d, 4s, and 4p Orbits   B015/B063

are given for illustration. There are 3 references: 1 Soviet and 2 US.

ASSOCIATION: Institut tonkoy khimicheskoy tekhnologii im. M. V.
               Lomonosova (Institute of Fine Chemical Technology imeni
               M. V. Lomonosov).
               Akademiya nauk SSSR Institut obshchey i neorganicheskoy
               khimii im. N. S. Kurnakova (Academy of Sciences USSR,
               Institute of General and Inorganic Chemistry imeni N. S.
               Kurnakov)

SUBMITTED: December 7, 1958

Card 2/2

5.3100
5.3700(B)
5(4)

68817

S/020/60/131/01/031/060
B011/B006

AUTHORS: Shustorovich, Ye. M., Dyatkina, M.Ye.

TITLE: The Electron Structures of Chromocene and Some Related Compounds

PERIODICAL: Doklady Akademii nauk SSSR, 1960, Vol 131, Nr 1, pp 113-116 (USSR)

ABSTRACT: The authors calculated the molecular orbitals (MO) of chromocene according to the method by S. S. J. Roothaan (Ref 2) in a generalized form for radicals (Ref 4) (since $(C_5H_5)_2Cr$ possesses unpaired electrons). The simplifications used in reference 1 were also applied in this calculation. The MO of $(C_5H_5)_2Cr$ and their energies are given in table 1. The authors give a scheme of the ground state of chromocene (A). The possibility of a different triplet state (B) in which the two unpaired electrons lie in a twofold degenerate level e_{2g} (higher than the level a'_{1g} occupied by one pair of electrons) is excluded since a self-consistent MO cannot be found for B. Since the calculated energies of the levels e_{2g} and a'_{1g} (-5.22 ev

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The Electron Structures of Chromocene and
Some Related Compounds

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B011/B006

and -4.02 ev) lie close to each other, the diamagnetic state
(see scheme V) must lie in immediate proximity of the ground
state. Thus it follows that the observed paramagnetism of
chromocene and the absence of an equilibrium between its para-
and diamagnetic forms are due to the difference in the energies
of the initial valence states and not to a great difference
in the energies of the higher occupied electron levels. These
valence states yield the corresponding molecular states A and
B (128 kcal and 167 kcal). The latter conclusion evidently
holds not only for chromocene, but also for other aromatic
complex compounds. In all the molecules investigated by the
authors, the higher occupied symmetry levels are e_{2g} and a'_{1g}.

The energies of these levels lie very close to each other. In
$(C_5H_5)_2Fe$ and $(C_5H_5)_2Co^+$ the e_{2g} levels are above the a'_{1g}
levels. In the chromium compounds, inversion occurs (probably
due to the greater influence of the donor bonds), so that e_{2g}
is lower than a'_{1g}. In aromatic complex compounds these

levels evidently verge on an accidental degeneracy (confirmed
by reference 6). Since there exist three levels, the energies

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The Electron Structures of Chromocene and
Some Related Compounds

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B011/B006

of which lie close to each other (two e_{2g} levels and one a'_{1g} level), the difference between the states characterized by different electron distributions in these levels must be very slight with respect to their MO energies. This confirms an assumption made previously by the authors, i.e., that the number of unpaired electrons in aromatic complex compounds is determined by the difference in the energies of the initial valence states. From the coefficients of the atomic orbitals in the MO of chromocene the following charge distribution is derived: +1.70 of the charge on the Cr atom and -0.17 on every C atom. Thus the Cr atom is much more highly charged than the Fe atom in ferrocene (+0.68). The essential difference in the properties of <u>ferrocene</u> and chromocene is connected with this fact. The similar magnitude of the charge on Cr in the bis-cyclopentadienyl compound on the one hand and the dibenzene compound on the other, together with the noticeably ionic character of chromocene allow the assumption that chromocene is a partly ionic molecule, in which the benzene rings play the

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The Electron Structures of Chromocene and
Some Related Compounds

S/020/60/131/01/031/060
B011/B006

part of the anions. There are 3 figures, 1 table, and 10 ref-
erences, 2 of which are Soviet.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii im. N. S. Kurnakova
Akademii nauk SSSR (Institute of General and Inorganic Chemistry
imeni N. S. Kurnakov of the Academy of Sciences, USSR)

PRESENTED: October 31, 1959, by I. I. Chernyayev, Academician

SUBMITTED: October 27, 1959

Card 4/4

5.3100

AUTHORS: Shustorovich, Ye. M., Dyatkina, M. Ye.

TITLE: The Electron Structure of the Ferricinium Cation and
              Other Aromatic Complex Compounds of Metals

PERIODICAL: Doklady Akademii nauk SSSR, 1960, Vol. 133, No. 1,
              pp. 141 - 143

TEXT: The authors calculated the molecular orbits (MO) of the ferri-
cinium cation (Table 1) by using the methods described in previous
papers (Refs. 1 and 2) and with the same approximations. Furthermore,
they describe the calculation of the MO of the cation $(C_6H_6)_2Cr^+$. They
were, however, unable to make a proper selection of structures. Never-
theless, they believe that the first structure (cf. Scheme) is more
probable. The authors also attempted a self-consistent calculation of
the molecules of $(C_5H_5)_2Co$ and $(C_5H_5)_2V$. They met with considerable dif-
ficulties and, therefore, had to restrict themselves to an estimate of
the effective charges. The authors met with major difficulties also in

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The Electron Structure of the Ferricinium Cation   81727
and Other Aromatic Complex Compounds of Metals   S/020/60/133/01/39/070
                                                   B011/B003

the case of the $(C_5H_5)_2V$ molecule; in this case, they only established
the electron configuration of the molecule $...(e_{2g})^2 (a'_{1g})^1$, and re-
stricted themselves to estimating the effective charges. Table 2 offers
the results obtained from the calculation of the effective charges on
the central atoms and on the rings in all molecules. These results are
discussed in the present and previous papers. The authors draw the fol-
lowing conclusions: The distribution of the electron density in the ca-
tions as compared to the corresponding neutral molecules corresponds to
the detachment of electrons from the rings, since the effective charge
of the central atom in all cations does not diverge much from the charge
in neutral molecules. Especially indicative are the most reliable data
on ferrocene (charge on Fe + 0.7, on the rings 0.35 each) and on the
ferricinium cation (+0.6 on Fe and +0.2 on the rings). This result fits
those obtained from experiments (according to A. N. Nesmeyanov and
E. G. Perevalov; not published). Calculations revealed that in the
$(C_6H_6)_2Cr^+$ cation the positive charge is concentrated on the central
atom, while the rings have a smaller negative charge. The latter is much

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The Electron Structure of the Ferricinium Cation   S/020/60/133/01/39/070
and Other Aromatic Complex Compounds of Metals   B011/B003

smaller than in dibenzene chromium, so that the passage of $(C_6H_6)_2Cr$ to
the cation must be accompanied by a weakening of the tendency toward
nucleophilic substitution. The high electron density in ferrocene- and
dibenzene chromium molecules and rings is in agreement with the aromatic
character of these complexes (Ref. 1). The high π-electron density be-
comes also manifest in that ferrocene (like benzene) forms molecular
compounds with the electron acceptors. It follows from Table 2 that in
the case of neutral bis-cyclopentadienyl compounds the effective posi-
tive charge on the central atom in the neutral $(C_5H_5)M$ molecules (Z)

rises during the early transition period in accordance with the strength-
ening of the ion character on the transition from vanadicene to chromo-
cene (Ref. 6). This tendency reaches its maximum in the case of
$(C_5H_5)_2Mn$, which is known to be an ion compound with a +2 charge on the
central atom. This is indicative of the presence of the five unpaired
electrons. A further addition of electrons leads to a rapid weakening
of the ion character in ferrocene, and especially in cobalticene. The
course taken by the charges is shown in Fig. 1. Finally, ruthenocene

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The Electron Structure of the Ferricinium Cation   81727
and Other Aromatic Complex Compounds of Metals   S/020/60/133/01/39/070
    B011/B003

and ruthenicinium are compared with ferrocene and ferricinium. The au-
thors did not receive the paper by R. E. Robertson and H. M. McConnel
(Ref. 9) until the time the slips were corrected, and they discuss it
therefore in an appendix. There are 1 figure, 2 tables, and 9 ref-
erences: 6 Soviet, 1 German, and 2 British.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii Akademii
    nauk SSSR (Institute of General and Inorganic Chemistry
    of the Academy of Sciences, USSR)

PRESENTED: March 3, 1960, by I. I. Chernyayev, Academician

SUBMITTED: March 1, 1960

Card 4/4

VOLKOV, V.M.; DYATKINA, M.Ye.

Structure of the complex ion $[OsNCl_5]^=$. Dokl.AN SSSR 134
no.2:351-353 S '60.
(MIRA 13:9)

1. Institut obshchey i neorganicheskoy khimii im. N.S.Kurnakova
Akademii nauk SSSR. Predstavleno akad. I.I. Chernyayevym.
(Osmium compounds)

20000

S/192/61/002/001/003/006
B101/B201

5.5700   2205 1164 1275 also 1160

AUTHORS: Shustorovich, Ye. M. and Dyatkina, M. Ye.

TITLE: Calculation of the ground states of dibenzene chromium,
              cobalticinium cation and chromocene by means of molecular
              orbits with self-consistence

PERIODICAL: Zhurnal strukturnoy khimii, v. 2, no. 1, 1961, 49-58

TEXT: Calculations have been made of the ground state of cobalticinium ca-
tion, $(C_5H_5)_2Co^+$, of dibenzene chromium, $(C_6H_6)_2Cr$, and of the chromocene,
$(C_5H_5)_2Cr$ by the method of C. C. J. Roothaan (Ref. 2, see below). The
authors proceeded from the following data: interval Co - C 2.10 A;
Cr - C 2.19 A; C - C 1.43 A; effective charge of the Slater orbits:
ζ_{2p} 1.6 for C; $\zeta_{4s, 4p}$ 0.8 for Cr, 1.1 for Co; ζ_{3d} 1.6 for Cr, 2.2 for Co$^+$.
Calculation results are given in Table 5: molecular orbits of the complexes
and molecular orbit energies. The lowest orbit is found to be the orbit of
a_{1g} symmetry, the highest with ferrocene and cobalticinium e_{2g}, with diben-

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20000

S/192/61/002/001/003/006
B101/B201

Calculation of ...

zene chromium and chromocene a'_{1g}. Levels e_{2g} and a'_{1g} have approximately
equal energies; thus, in accordance with the experimental data by
H. McConnell (Ref. 5. see below) all molecules possess three quasi-degener-
ate levels. Table 6 compares the calculated ionization potentials of
$(C_5H_5)_2Fe$ and $(C_5H_5)_2Cr$ with the measured ones. It is concluded from the
relatively good agreement between calculated and measured values that the
ionization potential of $(C_6H_6)_2Cr$ probably amounts to 4.19, and that of
$(C_5H_5)_2Co^+$ to 11.13 ev. Table 7 presents the distribution of electron
density, and Table 8 the allowed transitions. For ferrocene, the transition
energy was found to be equal to 2.88, 3.81, and 4.96 ev; for the cobalt-
icinium cation, it was equal to 3.10, 4.00, and 4.77 ev and in good agree-
ment with the ultraviolet spectra. S. N. Dobryakov is thanked for his as-
sistance in the calculations. There are 8 tables and 12 references:
4 Soviet-bloc and 8 non-Soviet-bloc. The 2 references to English language
publications read as follows: C. C. J. Roothaan, Rev. Mod. Phys., 23, 69,
(1951); H. McConnell, W. W. Borterfield, R. E. Robertson, J. Chem. Phys.,
30, 442. (1959).

Card 2/6

20000

S/192/61/002/001/003/006
B101/B201

Calculation of ...

ASSOCIATION: Moskovskiy institut tonkoy khimicheskoy tekhnologii im. M. V.
Lomonosova (Moscow Institute of Fine Chemical Technology imeni
M. V. Lomonosov); Institut obshchey i neorganicheskoy khimii
AN SSSR im. N. S. Kurnakova (Institute of General and Inorganic
Chemistry imeni N. S. Kurnakov of AS USSR)

SUBMITTED: February 14, 1960

Legend to Table 5: 1) symmetry; 2) molecule; 3) binding molecular orbits;
a) type of orbit; b) energy (ev); 4) loosening orbits
Legend to Table 6: 1) potential; 2) calculated; 3) measured
Legend to Table 7: 1) compound; 2) effective charges (in atomic units);
a) at the central atom; b) at both rings; c) at one ring; d) at every C atom;
3).dipole moments (in D); e) bond metal - C; f) metal - ring
Legend to Table 8: 1) single electron transition; 2) excited states of the
molecules; a) orbital degeneracy (without consideration of electron - elec-
tron interaction); b) symmetry of the states (under consideration of elec-
tron - electron interaction); 3) allowed transitions.

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S/192/61/002/001/003/006

Calculation of

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① Симметрия	⑤ Молекула	③ Связывающие МО		② Разрыхляющие МО
		⑥ Вид орбиты	④ Энергия (ээ)	④ Энергия (ээ)
a_{1g}	$Co(C_5H_5)_2^+$ $Cr(C_5H_5)_2$ $Cr(C_6H_6)_2$	$0,79a_{1g} + 0,62s$ $0,97a_{1g} + 0,25s$ $0,98a_{1g} + 0,22s$	$-20,84$ $-13,71$ $-13,31$	$-5,33$ $+1,74$ $+3,21$
a'_{1g}	$Co(C_5H_5)_2^+$ $(Cr C_5H_5)_2$ $Cr(C_6H_6)_2$	d_{z^2} d_{z^2} d_{z^2}	$-13,20$ $-4,82$ $-4,19$	— — —
a_{1u}	$Co(C_5H_5)_2^+$ $Cr(C_5H_5)_2$ $Cr(C_6H_6)_2$	$0,91a_{1u} + 0,41p_z$ $0,99a_{1u} + 0,06p_z$ $0,99a_{1u} + 0,062p_z$	$-18,04$ $-13,12$ $-12,73$	$-5,20$ $+3,73$ $+2,15$
e_{1u}	$Co(C_5H_5)_2^+$ $Cr(C_5H_5)_2$ $Cr(C_6H_6)_2$	$0,77e_{1u} + 0,64p_x$ $0,94e_{1u} + 0,35p_x$ $0,94e_{1u} + 0,36p_x$	$-16,65$ $-9,82$ $-10,72$	$-1,96$ $+4,05$ $+3,94$
e_{1g}	$Co(C_5H_5)_2^+$ $Cr(C_5H_5)_2$ $Cr(C_6H_6)_2$	$0,90e_{1g} + 0,44d_{xz}$ $0,92e_{1g} + 0,39d_{xz}$ $0,98e_{1g} + 0,30d_{xz}$	$-14,20$ $-10,56$ $-10,61$	$+0,19$ $+7,94$ $+10,12$
e_{2g}	$Co(C_5H_5)_2^+$ $Cr(C_5H_5)_2$ $Cr(C_6H_6)_2$	$0,32e_{2g} + 0,95d_{xy}$ $0,55e_{2g} + 0,83d_{xy}$ $0,78e_{2g} + 0,63d_{xy}$	$-11,13$ $-5,22$ $-4,76$	$+0,57$ $+5,88$ $+6,97$
e_{2u}	$Co(C_5H_5)_2^+$ $Cr(C_5H_5)_2$ $Cr(C_6H_6)_2$	e_{2u} e_{2u} e_{2u}	— —	$-0,25$ $+4,00$ $+2,19$

Calculation of ...

(1) Потенциал	(C₅H₅)₂Fe	(C₅H₅)₂Cr
(9) Вычисленный	6,39	4,82
(10) Измеренный	7,05	6,90

Table 4

(1) Соединение	(2) Эффективные заряды (в атомных единицах)				Дипольные моменты (3) (в D)	
	на центральном атоме (a)	на обоих кольцах (b)	на одном кольце (c)	на каждом атоме С (d)	(e) связи металл—С	металл—(f) кольцо
(C₆H₆)₂Cr	+1,470	—1,470	—0,735	—0,122	1,30	5,90
(C₅H₅)₂Fe	+0,682	—0,682	—0,341	—0,068	0,57	2,64
(C₅H₅)₂Cr	+1,700	—1,700	—0,850	—0,170	1,80	7,40
(C₅H₅)₂Co⁺	—0,118	+1,118	+0,559	+0,112		

Card 5/6

Calculation of ...

Table 8

(A) Одно-электронный переход $\varphi_i \to \varphi_a$	(B) Возбужденные состояния молекул		(E) Разрешенные переходы
	(C) Орбитальное вырождение	(D) Симметрия состояний	
$e_{2g} \to e'_{1u}$	4	$E_{1u} + E_{2u}$	$^1A_{1g} \to {}^{1,3}E_{1u}$
$e_{2g} \to e_{2u}$	4	$A_{1u} + A_{2u} + E_{1u}$	$^1A_{1g} \to {}^{1,3}A_{1u}\ {}^{1,3}E_{1u}$
$a'_{1g} \to a'_{1u}$	1	A_{1u}	$^1A_{1g} \to {}^{1,3}A_{1u}$
$a'_{1g} \to e'_{1u}$	2	E_{1u}	$^1A_{1g} \to {}^{1,3}E_{1u}$

Card 6/6

S/078/61/006/003/010/022
B121/B208

AUTHORS: Dyatkina, M. Ye., Markov, V. P., Tsapkina, I. V., Mikhaylov,
             Yu. N.

TITLE: Electron structure of the group UO_2 in uranyl compounds

PERIODICAL: Zhurnal neorganicheskoy khimii, v. 6, no. 3, 1961, 575-580

TEXT: The stability of the uranyl group in various compounds depends on the
remaining atoms or groups appearing as addenda in the coordination sphere of
uranyl. The uranium atom is characterized by a large number of free elec-
tron orbits. There are donor-acceptor bonds between the ligands and uranium,
which compete with the donor-acceptor bonds of the UO_2 group. This competi-
tion results in the formation of solid complexes of uranium with ligands of
pronounced donor properties, such as ammonia, amines, thiourea, etc. The
formation of secondary bonds between uranium and the ligands also depends
largely on their ionic character. The nature of the bonds in the compounds
UF and UO_2F is discussed. The existence of donor-acceptor bonds with sec-
ondary ligands prevents the appearance of additional donor-acceptor bonds of
U with oxygen. By substituting H_2O or $CO(NH_2)_2$ for the secondary ligands

Card 1/2

Electron structure ...

S/078/61/006/003/010/022
B121/B208

NO_3', C_2O_4'' or SO_4'', the number of donor-acceptor bonds is increased and the donor-acceptor bonds in the $\overleftarrow{U{=}O}$ group are weakened. The ν_{asUO_2} frequency thus decreases. This decrease occurs by strengthening the donor properties of the secondary ligands in uranium compounds. This result agrees with the observation made by V. M. Vdovenko, D. N. Suglobov, and V. A. Krasil'nikov (Ref. 12). The change of paramagnetic susceptibility by inclusion of secondary ligands is discussed. By exchanging H_2O for $CO(NH_2)$ in the sulfates, chlorides, and oxalates of uranyl, the paramagnetic susceptibility is slowly increased. The authors also discuss the change of the polarizability of the uranyl ion by inclusion of acceptor-donor ligands. The competition between the donor-acceptor bonds of the UO_2 group and secondary ligands is observed in the following groups: NpO_2, PuO_2, AmO_2, TiO, ZrO, VO, etc.

Mention is made of Ya. K. Syrkin, V. I. Belov, A. N. Nesmeyanov, and T. P. Tolstaya. There are 17 references: 7 Soviet-bloc and 10 non-Soviet-bloc.

SUBMITTED: September 21, 1960

Card 2/2

SHUSTOROVICH, Ye.M.; DYATKINA, M.Ye.

Effective charge on the Ni atom in the nickelecinium cation.
Zhur.neorg.khim. 6 no.5:1247-1248 My '61.   (MIRA 14:4)

(Nickel compounds)

/l. 440 C

AUTHORS: Shustorovich, Ye. M. and Dyatkina, M. Ye.

TITLE: Electronic structure of the ferrocene molecule

PERIODICAL: Zhurnal strukturnoy khimii, v.3, no. 3, 1962, 345-346

TEXT: The authors compare data previously obtained by them (Ye.M.
Shustorovich et al, Dokl. AN SSSR, 128, 1234, 1959) about the elec-
tronic structure of the ferrocene molecule $(C_2H_5)_2Fe$, with those
of the Danish scientists J. P. Dahl and C. J. Ballhausen, in order
to verify the results of both sets of calculations. The items dis-
cussed include: The ionization potential; the electron density
distribution; the energy of the $3d_{z^2}$ orbit; the MO sequence; and
the energies of single electron transfers. They conclude that their
calculations agree best with the experimental evidence.

Inst. Gen & Inorganic Chem, AS USSR

Card 1/2

MOROZOVA, I.D.; DYATKINA, M.Ye.

Spin density distribution in some metal ketyls.
Dokl. AN SSSR 146 no.4:830-832 O '62.   (MIRA 15:11)

1. Institut organicheskoy khimii AN SSSR, g. Kazan',
Predstavleno akademikom B.A. Arbuzovym.
        (Ketyls—Spectra)   (Molecular orbitals)

DYATKINA, M.Ye.; MIKHAYLOV, Yu.N.

Structure of uranyl and its analogs. Zhur.strukt.khim. 3
no.6:724-747 '62.   (MIRA 15:12)

1. Institut ôbshchey i neorganicheskoy khimii imeni Kurnakova
AN SSSR.
   (Uranyl compounds)   (Crystallography)   (Molecular orbitals)

VOLKOV, V.M.; DYATKINA, M.Ye.

Locating the best σ - and π-orbitals by the method of maximum overlap. Zhur.strukt.khim. 4 no.4:610-616 Jl-Ag '63. (MIRA 16:9)

1. Institut obshchey i neorganicheskoy khimii imeni Kurnakeva.
        (Valence (Theoretical chemistry)) (Molecular orbitals)

VOLKOV, V.M.; DYATKINA, M.Ye.

Determination of the most stable configuration of molecules
by the method of maximum overlap. Zhur.strukt.khim. 4 no.5:
728-733 S-O '63.   (MIRA 16:11)

1. Institut obshchey i neorganicheskoy khimii imeni N.S. Kurnakova
AN SSSR.

LEVIN, A.A.; VOLKOV, V.M.; DYATKINA, M.Ye.

Theoretical examination of the stereochemistry of complex compounds
of elements with F-electrons. Part 1: Conversion of the f-orbital
of the central atom. Zhur.strukt.khim. 4 no.6:930-934 N-D '63.
(MIRA 17:4)

1. Institut obshchey i neorganicheskoy khimii imeni Kurnakova
AN SSSR.

DYATKINA, M.Ye.

"Chemical bonds in complex compounds" by I.B. Bersuker, A.V.
Ablov. Reviewed by M.E. Diatkina. Zhur. neorg. khim. 8 no.7:
1797-1798 Jl '63.   (MIRA 16:7)

(Complex compounds)   (Chemical bonds)
(Bersuker, I.B.)   (Ablov, A.V.)

VOLKOV, V.M.; DYATKINA, M.Ye.

Participation of an unshared pair of electrones in hybridisation.
Zhur. neorg. khim. 8 no.8:1820-1825 Ag '63.   (MIRA 16:8)

1. Institut obshchey i neorganicheskoy khimii imeni Kurnakova
AN SSSR, laboratoriya stroyeniya neorganicheskikh soyedineniy.
          (Molecular orbitals)   (Hybrides)

MOROZOVA, I.D.; DYATKINA, M.Ye.

Spin density distribution in aromatic metal ketyls. Dokl. AN SSSR
150 no.2:337-339 My '63.   (MIRA 16:5)

1. Institut organicheskoy khimii AN SSSR v.g. Kazani i Institut
obshchey i neorganicheskoy khimii im. N.S.Kurnakova AN SSSR.
Predstavleno akademikom B.A.Arbuzovym.
    (Organometallic compounds)   (Molecular orbitals)

VOLKOV, V.M.; LEVIN, A.A.; DYATKINA, M.Ye.

On the relative stability of isomers in MX_2Y_2 molecules.
Dokl. AN SSSR 152 no.2:359-362 S '63.   (MIRA 16:11)

1. Institut obshchey i neorganicheskoy khimii im. N.S. Kurnakova
AN SSSR. Predstavleno akademikom I.I. Chernyayevym.

GOLOVNYA, V.A., doktor khim. nauk; ELLERT, G.V., kand. khim. nauk;
    SHUBOCHKIN, L.K., kand. khim. nauk; SHCHELOKOV. R.N., kand.
    khim. nauk; TSAPKINA, I.V., kand. khim. nauk; TRAGGEYM, Ye.N.,
    kand. khim. nauk; MARKOV, V.P., doktor khim. nau, [deceased];
    ALTKHANOVA, Z.M.; DYATKINA, M.Ye.. doktor khim. nauk; MIKHAYLOV,
    Yu.N.; TSAPKIN,V.V.,kand.khim.nauk; BOLOTOVA,G.T.,kand.khim.nauk;
    CHERNYAYEV,V.A.,doktor khim.nauk; KORCHEMNAYA,Ye.K., red.

    [Complex compounds of uranium] Kompleksnye soedineniia urana.
    Moskva, Izd-vo "Nauka," 1964.   488 p.   (MIRA 17:7)

    1.Akademiya nauk SSSR. Institut obshchey i neorganicheskoy
    khimii. 2. Laboratoriya khimii kompleksnykh soyedineniy ak-
    tinidov Instituta obshchey i neorganicheskoy khimii AN SSSR
    (for all except Korchemnaya).

_DYATKINA, M.Ye.; MIKHAYLOV, Yu.N.

    Nature of the Re-O bond in K ReO (CN). Zhur.strukt.khim.
    5 no. 2:325 Mr-Ap '64.   (MIRA 17:6)

    1. Institut obshchey i neorganicheskoy khimii imeni N.S.
    Kurnakova AN SSSR.

VOLKOV, V.M.; DYATKINA, M.Ye.

Theoretical study of the stereochemistry of complex compounds
with f-electrons. Part 2: Determination of the most stable
configuration of the $Th(NCS)_8^{4-}$ ion by the method of maximum
overlap. Zhur. strukt. khim. 5 no.4:611-619 Ag '64.

(MIRA 18:3)

1. Institut obshchey i neorganicheskoy khimii imeni Kurnakova
AN SSSR.

LEVIN, A.A.; VARYUSHCHENKO, L.I.; DYATKINA, M.Ye.

Application of the variation-iteration method for the
determination of the most stable configuration of MX_k
molecules. Part 1: Molecules of MX_4 in approximation of
σ-bonds. Zhur. strukt. khim. 5 no.4:654-655 Ag '64.

(MIRA 18:3)

1. Institut obshchey i neorganicheskoy khimii imeni Kurnakova
AN SSSR.

CHARKIN, O.P.; DYATKINA, M.Ye.

Geometric structure of halide, of elements of group 3 of the
periodic table. Zhur. strukt. khim. 5 no.6:921-923 N-D '64.

(MIRA 18:4)

1. Institut obshchey i neorganicheskoy khimii imeni Kurnakova
AN SSSR.

CHARKIN, O.P.; DYATKINA, M.Ye.

Geometric structure of halides and oxides of elements of group 4 of
the periodic table. Zhur. strukt. khim. 5 no.6:924-927 N-D '64.
                                                    (MIRA 18:4)

MOROZOVA, I.D.; DYATKINA, M.Ye.

Spin density distribution in metal ketyls containing methyl groups.
Dokl. AN SSSR 154 no. 3:687-689 Ja '64.   (MIRA 17:5)

1. Institut organicheskoy khimii AN SSSR, Kazan', i Institut
obshchey i neorganicheskoy khimii im. N.S.Kurnakova AN SSSR.
Predstavleno akademikom B.A.Arbuzovym.

CHARKIN, O..P.; DYATKINA, M.Ye.

Calculation of the Slater-Kondon parameters from atomic spectra
for atoms and ions of the second and third transition periods.
Zhur. strukt. khim. 5 no.3:440-450 My-Je '64.

Geometry of halides of elements of the second group of a periodic
table. Ibid.:451-454   (MIRA 18:7)

1. Institut obshchey i neorganicheskoy khimii imeni N.S. Kurnakova
AN SSSR.

MOROZOVA, I.D.; DYATKINA, M.Ye.

Negative spin density in methyl ketyls. Zhur. strukt. khim. 6 no.2:
278-282 Mr-Ap '65.   (MIRA 18:7)

1. Institut organicheskoy khimii AN SSSR, Kazan' i Institut obshchey
i neorganicheskoy khimii imeni Kurnakova AN SSSR.

IONOVA, G.V.; DYATKINA, M.Ye.

    Molecular orbitals of tetrahedral transition metal oxyanions. Report
    No.3: Orthovanadate ion. Zhur. strukt. khim. 6 no.2:283-285 Mr-Ap
    '65.   (MIRA 18:7)

    1. Institut obshchey i neorganicheskoy khimii imeni Kurnakova AN
    SSSR.

CHARKIN, O.P.; DYATKINA, M.Ye.

Calculation of the affinity to electron of transition elements
by the gloculer method. Zhur. struk. khim. 6 no.3:422-435 My-Je
'65.   (MIRA 18:8)

1. Institut obshchey i neorganicheskoy khimii imeni N.S.Kurnakova
AN SSSR.

KLIMENKO, N.M.; KRYLOVA, Ye.N.; MIKHALEVA, N.M.; CHURIKOV, Yu.I.; DYATKINA, M.Ye.

Computation of dicentric Coulomb integrals including 3d-, 4s-, and
4p orbitals. Zhur. struk. khim. 6 no.3:407-421 My-Je '65.

(MIRA 18:8)

1. Institut obshchey i neorganicheskoy khimii imeni N.S.Kurnakova
AN SSSR i Moskovskiy institut tonkoy khimicheskoy tekhnologii imeni
M.V.Lomonosova.

IONOVA, G.V.; DYATKINA, M.Ye.

Molecular orbits of MnO_3F. Zhur. neorg. khim. 10 no.9:2036-2040 S
'65.   (MIRA 18:10)

1. Institut obshchey i neorganicheskoy khimii imeni Kurnakova AN SSSR.

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BUSLAYEV, Yu.A.; SHCHERBAKOV, V.A.; DYATKINA, M.Ye.

Nuclear magnetic resonance of F^{19} in the solution of
fluorides of the elements of the group IV. Zhur. strukt.
khim. 6 no.1:16-20 Ja-F '65.

(MIRA 18:12)

1. Institut obshchey i neorganicheskoy khimii imeni N.S.
Kurnakova AN SSSR i Radiyevyy institut imeni V.G. AN SSSR,
Leningrad. Submitted August 22, 1964.

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Molecular orbits of tetrahedral hydroxyanions of transition
elements. Report No.1: Chromate and permanganate. Zhur. strukt.
khim. 6 no.1:128-136 Ja-F '65.

(MIRA 18:12)

1. Institut obshchey i neorganicheskoy khimii imeni N.S.
Kurnakova AN SSSR. Submitted January 10, 1964.

DYATKINA, M.Ye.; CHARKIN, O.P.

Valence state energies in the inert gas compounds and certain
other halides. Zhur. strukt. khim. 6 no.1:174-176 Ja-F '65.
                                              (MIRA 18:12)
1. Institut obshchey i neorganicheskoy khimii imeni N.S.
Kurnakova AN SSSR. Submitted October 10, 1964.

KLIMENKO, N.M.; DYATKINA, M.Ye.

Calculation of two-center molecular integrals including
ns-, np-, and nd-atomic orbitals. Zhur.strukt.khim. 6
no.5:755-764 S-O '65.   (MIRA 18:12)

1. Institut obshchey i neorganicheskoy khimii imeni N.S.
Kurnakova AN SSSR i Moskovskiy institut tonkoy khimicheskoy
tekhnologii imeni M.V.Lomonosova. Submitted December 12, 1964.

IONOVA, G.V.; DYATKINA, M.Ie.

Molecular orbitals of tetrahedral oxyanions of transition metals.
Report No.4: FeO$_4$ molecule. Zhur.strukt.khim. 6 no.5:796-797
S-O '65.   (MIRA 18:12)

1. Institut obshchey i neorganicheskey khimii imeni N.S.Kurnakova,
AN SSSR. Submitted March 1, 1965.

CHARKIN, O.P.; DYATKINA, M. Ye.

Valence state energies of transition metal atoms in gaseous
molecules of halides MX. Part 1: Dihalides, MX$_2$. Zhur. strukt. khim.
6 no. 4:579-590 Jl-Ag '65   (MIRA 19:1)

1. Institut obshchey i neorganicheskoy khimii imeni N.S. Kurnakova
AN SSSR. Submitted January 30, 1965.

KLIMENKO, N.M.; DYATKINA, M. Ye.

Calculation of auxiliary functions $C_{\alpha\beta}^{\gamma\delta\epsilon}$ (Pa,Pb), occurring in the determination of two-center molecular integrals for the arbitrary Λ. Zhur. strukt. khim. 6 no. 4:604-613 Jl-Ag '65
(MIRA 19:1)

1. Institut obshchey i neorganicheskoy khimii imeni N.S. Kurnakova AN SSSR i Moskovskiy institut tonkoy khimicheskoy tekhnologii imeni M.V. Lomonosova. Submitted December 12, 1964.

GERMAN, E.D.; LEVIN, A.A.; DYATKINA, M. Ye.

Spin-orbital interaction with self-consistency for molecules
with open shells. Zhur. strukt. khim. 6 no. 4:614-618 Jl-Ag '65
                                              (MIRA 19:1)
1. Institut obshchey i neorganicheskoy khimii imeni N.S. Kurnakova
AN SSSR. Submitted December 30, 1964.

L 9898-63   EWP(q)/BDS/EWT(m)—AFFTC—JD/WB
ACCESSION NR: AP3000412   S/0076/63/037/005/1037/1042

AUTHOR: Tsvetnova, R. V.; Dyatkina, S. L.; Sheremet'yeva, S. N.; Kel'n, A. R.;
Krasil'shchikov, A. I.

58

TITLE: Corrosion and passivity of titanium in sulfuric acid solution   57

SOURCE: AN SSSR. Zhurnal fizicheskoy khimii, v. 37, no. 5, 1963, 1037-1042

TOPIC TAGS: corrosion, passivity of titanium, electrochemical behavior of Ti;
passivating adsorption layer

ABSTRACT: The electrochemical and corrosion behavior of Ti in 5 and 10 N
sulfuric acid solutions, alone and in the presence of additions of potassium
iodide, tetraethylammonium iodide, copper sulfate and nitric acid, in a
nitrogen atmosphere, has been investigated by the potentiometric and discharge
curve methods, as well as by gravimetric determination of the corrosion losses.
Passivation is impeded by raising the temperature. The addition of I sup -,
Cu sup 2+ and HNO sub 3 retards anodic solution of Ti in H sub 2 SO sub 4 and
facilitates initial passivation of the metal. It is suggested that the

Card 1/2

L 9898-63
ACCESSION NR: AP3000412

passivity of Ti is due to the formation of a passivating adsorption layer on its surface. Orig. art. has: 3 equations, 1 table, 8 figures.

ASSOCIATION: Gosudarstvenniy nauchno-issledovatel'skiy i proektniy institut azotnoy promy*shlennosti (State Scientific Research and Design Institute for Nitrogen Industry)

SUBMITTED: 22Jan62   DATE ACQ: 18Jun63   ENCL: 00

SUB CODE: 00   NR REF SOV: 011   OTHER: 006

Card 2/2